Mark J Abraham

List of Publications by Year
in descending order

9 papers	15,781 citations	1162889 8 h-index	1474057 9 g-index
10 all docs	10 docs citations	10 times ranked	20623 citing authors

#	Article	IF	Citations
1	Heterogeneous parallelization and acceleration of molecular dynamics simulations in GROMACS. Journal of Chemical Physics, 2020, 153, 134110.	1.2	275
2	Sharing Data from Molecular Simulations. Journal of Chemical Information and Modeling, 2019, 59, 4093-4099.	2.5	26
3	Trends in Data Locality Abstractions for HPC Systems. IEEE Transactions on Parallel and Distributed Systems, 2017, 28, 3007-3020.	4.0	61
4	Tackling Exascale Software Challenges in Molecular Dynamics Simulations with GROMACS. Lecture Notes in Computer Science, 2015, , 3-27.	1.0	581
5	GROMACS: High performance molecular simulations through multi-level parallelism from laptops to supercomputers. SoftwareX, 2015, 1-2, 19-25.	1.2	14,414
6	Direct-Space Corrections Enable Fast and Accurate Lorentzâ€“Berthelot Combination Rule Lennard-Jones Lattice Summation. Journal of Chemical Theory and Computation, 2015, 11, 5737-5746.	2.3	112
7	Performance enhancements for GROMACS nonbonded interactions on BlueGene. Journal of Computational Chemistry, 2011, 32, 2041-2046.	1.5	8
8	Optimization of parameters for molecular dynamics simulation using smooth particleâ€mesh Ewald in GROMACS 4.5. Journal of Computational Chemistry, 2011, 32, 2031-2040.	1.5	217
9	Ensuring Mixing Efficiency of Replica-Exchange Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2008, 4, 1119-1128.	2.3	71